Study of the Chemical Properties of RDX High-Energy Element and its Derivatives with Different Nanostructures of Mass by Functional Density Theory

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Abstract

In this research, RDX energy derivatives with different carbon nanoparticles under different temperature conditions were studied using density functional theory. For this purpose, the materials were first geometric optimized, then the thermodynamic parameters were calculated for all of them. Then, the process of changing the energy-dependent parameters such as specific heat capacity, enthalpy, entropy and Gibbs free energy relative to molecular mass, molecular volume and measured level in this study at a given temperature, were evaluated against each other.

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Keywords: High Energy Energy Derivatives, Different Carbon Fullerenes, RDX, Functional Density Theory.

1. Introduction

The methylene trietramine cyclotryl RDX is a high energy source, the easiest way to increase the amount of hexamethylene tetramine to an excess of nitric acid at 25 ° C and heat it up to 55 ° C. The RDX is deposited with cold water and then the mixture is boiled to remove any soluble impurities. Purification of RDX is done by acetone crystallization. During World War II, it was not used as the main filler in shells and bombs, but was added to TNT in order to increase the power of explosive components. RDX was used in Germany, France, Italy, Japan, Russia, the United States, Spain and Sweden in explosive devices. R & D continued to advance new and much more powerful explosives during World War II. Trpx (AI / RDX / TNT) and cyclo-tetramethylene tetranitramine, known as octogen ($C_4H_8N_8O_8$) (HMX), were available at the end of World War II. In 1952, an explosive blend called "octole" was developed. Explosive compounds used are of the type of green fuels and do not cause pollution in the environment [1-5]. In this research, RDX derivatives with different carbon nanotubes in different temperature conditions were studied using density functional theory.
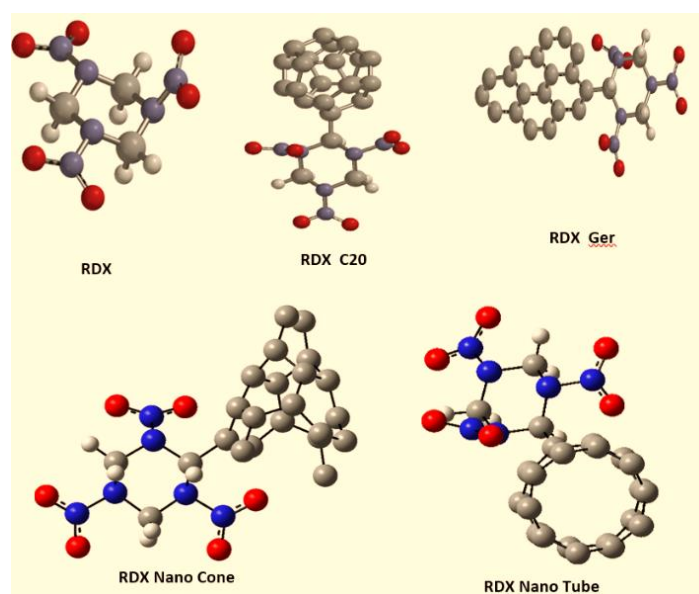

Fig1. Optimized images of RDX molecules and their derivatives with different nanostructures, with the same carbon number

Table 1). Some chemical properties calculated at B3lyp / 6-31g levels for RDX derived derivatives with different carbon nanoparticles

	Temperature=298.15K , pressure=1 atm				
	RDX	**RDX C$_{20}$**	**RDX NanoCone**	**RDX Ger**	**RDX Nano Tube**
ENERGY(au)	-880.703152	-1627.18088	-1625.67721	-1589.53055	-1625.71283
E HOMO(eV)	-8.63	-10.66	-9.84	-8.54	-9.14
E LUMO (eV)	5.13	-3.95	-2.46	-3.69	-4.59
Dipole Moment (debye)	3.60	13.26	13.99	24.54	9.35
Weight(amu)	222.117	461.329	461.329	449.318	461.329
Volume(A^3)	160.53	367.09	411.91	386.19	421.93
Area (A^2)	192.71	344.46	398.56	387.64	378.32
ZPE (KJ/mol)	427.43	744.09	623.71	680.64	574.80
H° (au)	-880.528656	-1626.87988	-1625.41499	-1589.24977	-1625.46704
CV (J/mol)	186.55	331.79	448.57	390.12	489.66
S° (J/mol)	433.17	542.89	657.01	610.14	692.24
G° (au)	-880.577846	-1626.94153	-1625.48960	-1589.31906	-1625.54570

2 .Calculations and results:

A computational study for RDX derived derivatives with different carbon nanotubes was studied using density functional theory. This operation was performed using Gaussian 98 and Gossive software. The compounds were first optimized by density functional theory method in the base series (6-31g). Then, IR studies were performed to calculate the thermodynamic parameters related to the process. All calculations at B3lyp / 6-31g levels of 300 to 400 degrees Kelvin and pressure ΔΠ atmosphere has been done. The results of the calculations showed that by increasing the molecular mass, molecular volume and molecular surface of the RDX material, the explosive derivatives with different nanostructures increase the carbon content of the specific heat capacity, and, of course, the internal energy also decreases. Fig. 2- 4 [6-10].
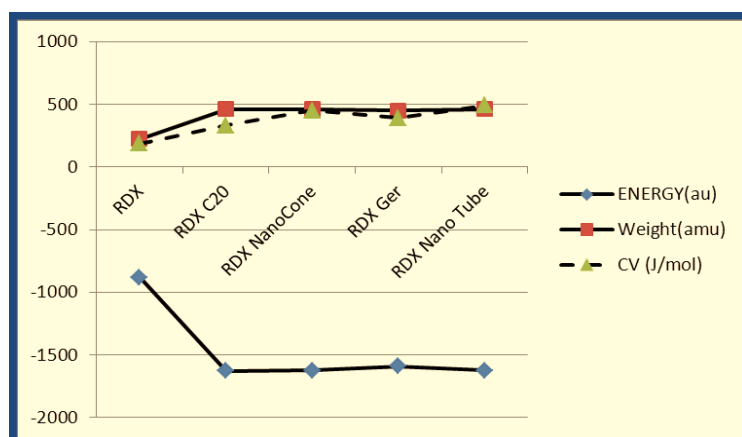

Fig 2 Comparison of the molecular mass, internal energy and specific heat capacity of the RDX explosive and its derivatives with different carbon nanoparticles.
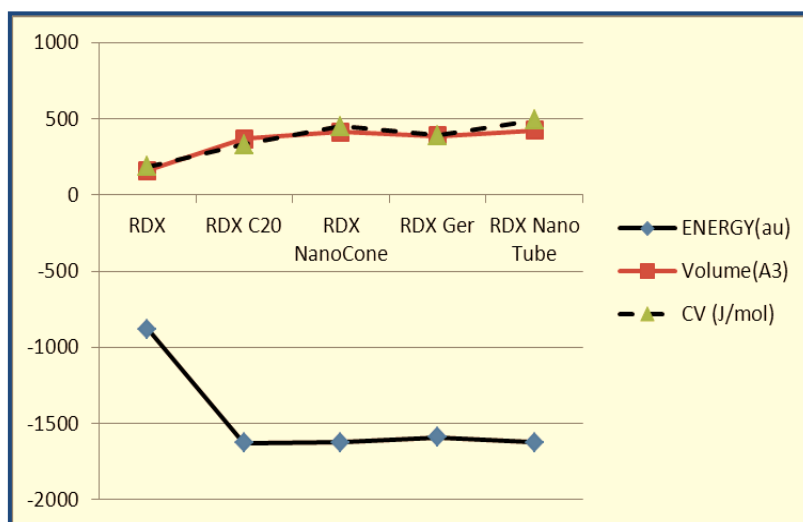
Fig3. Comparison of the molecular volume, internal energy and specific heat capacity of the RDX explosive and its derivatives with different carbon nanostructures.
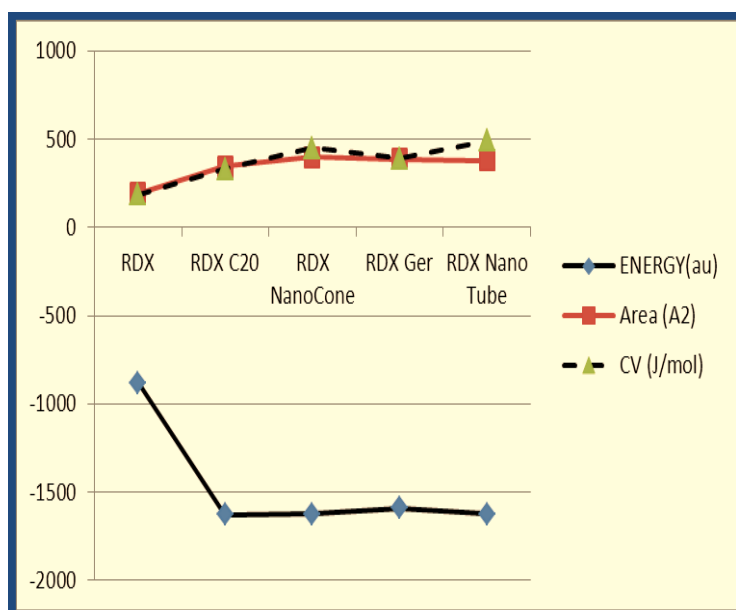

Figure 4: Comparison of the molecular level, internal energy and specific heat capacity of the RDX explosive and its derivatives with different carbon nanotubes.

Also, the results of the calculations showed that with increasing molecular mass, the RDX material to the derivatives of explosives with different nanostructures with carbon has the same specific heat capacity, but increasing the molecular mass of molten enthalpy and free energy of molybdenum gibes decreases. Figure 5- 6. Also, the study of molar entropy showed that with increasing molecular mass, molecular volume and

molecular surface, RDX material increases to derivatives of explosives with similar nano-structures with similar carbon (Fig. 7).[11-12]
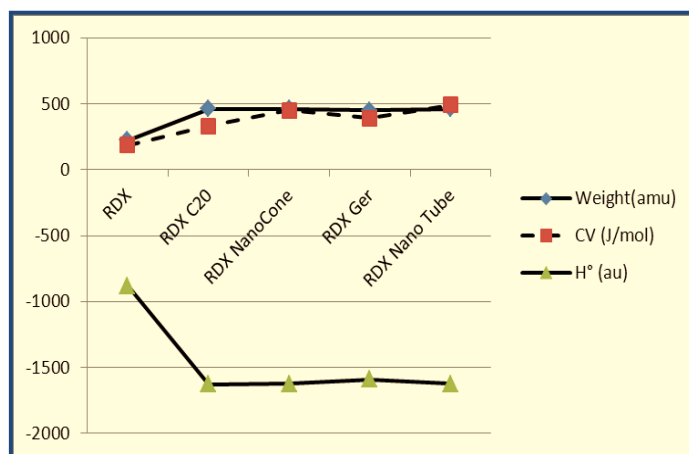

Fig 5 The comparison of molecular enthalpy, molecular mass and specific heat capacity of the RDX explosive and its derivatives with similar carbon nanotubes
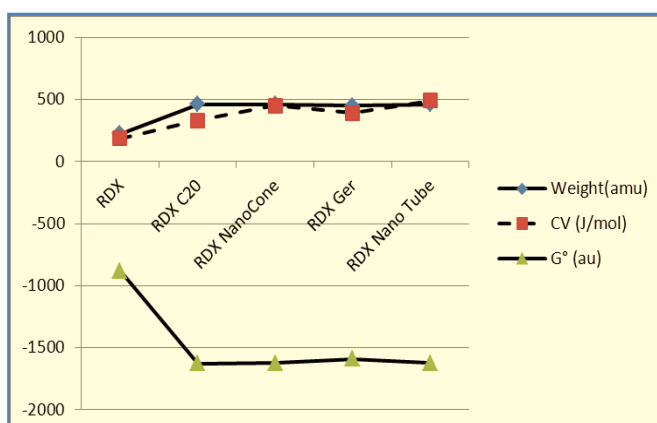

Fig. 6 Graph of Molybdenum Gibbs Free Energy, Molecular Mass and Special Heat Capacity of RDX Explosives and its Derivatives With different nano-structures, the same carbon is used
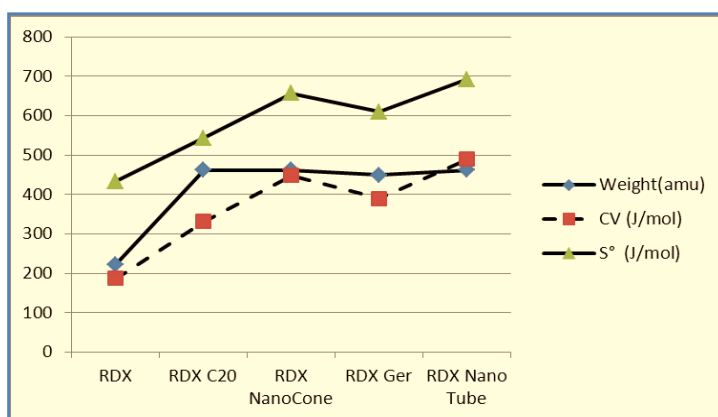

Fig. 7 Chart of the molecular entropy, molecular mass and specific heat capacity of the RDX explosive and its derivatives with similar carbon nanotubes

3. Calculate and test the specific heat capacity of CV at different temperatures

Using the Gaussian 98 program, the specific CV-specific CV values for RDX explosives and their derivatives with different carbon nanoparticles used in this study were calculated at a temperature range of 300 to 400 degrees Celsius every 10 degrees.

Table 3: Specific heat capacity variations for RDX explosives and their derivatives with different carbon nanotubes, used at temperatures

|	Cv(J/mol.K)				
Temperature	RDX	RDX C20	RDX NanoCone	RDX Geraphene	RDX Nano Tube
300	187.2671	333.7288	450.3865	391.7757	491.5348
310	191.1575	344.1805	460.1052	400.6579	501.5103
320	195.0306	354.5894	469.6509	409.429	511.2446
330	198.8871	364.9433	479.0256	418.0913	520.7422
340	202.727	375.2304	488.2314	426.6468	530.0078
350	206.5499	385.4403	497.2699	435.0964	539.0466
360	210.355	395.5628	506.1427	443.4411	547.8633
370	214.1412	405.5888	514.8511	451.6809	556.4631
380	217.9069	415.5098	523.3964	459.8156	564.8508
390	221.6505	425.3182	531.7796	467.8448	573.0314
400	225.3701	435.007	540.0019	475.7676	581.0096
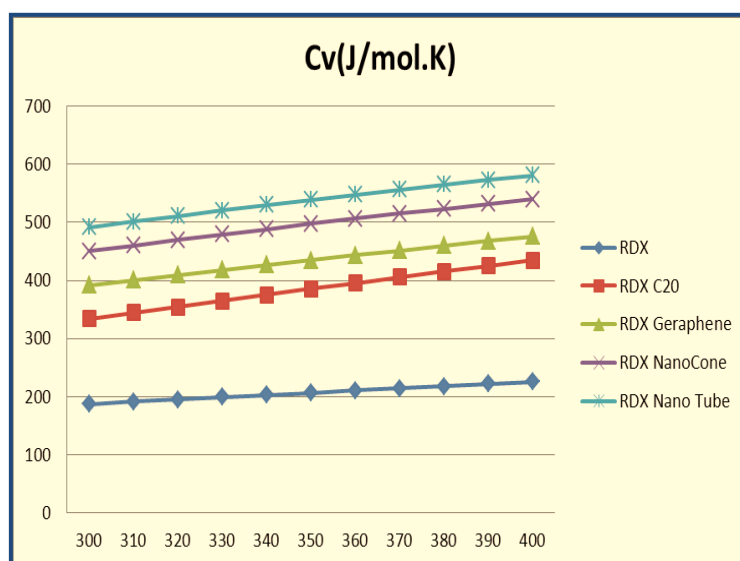
Fig 8. Chart of CV Specific Heat Capacity Changes for RDX Explosives and its Derivatives with Different Nanostructures with Similar Carbons Used at Different Temperatures

Changes in the specific CV heat capacity values in an RDX explosive and its derivatives with different carbon nanotubes, used at various temperatures, show that adding nano structures to RDX explosives at different temperatures has a specific heat capacity of CV in all cases relative to The raw material has been increased, and on the other hand, in all cases examined by increasing the temperature, the specific heat capacity of the CV increases (Fig. 8).

4. Discussion and Conclusion

The results of the calculations show that the RDX explosive after adding different nanostructures with the same carbon number to the specific heat capacity of the derivatives is increased. On the other hand, various derivatives, due to the increase in their specific heat capacity at different temperatures, The following are shown:

$$Cv_{\text{RDX Nano Tube}} > Cv_{\text{RDX Nano Cone}} > Cv_{\text{RDX Ger}} > Cv_{\text{RDX C20}} > Cv_{\text{RDX}}$$

Since the number of carbon in the nanostructures used in this study is considered to be the same, the molecular mass of the resulting derivatives is equal, but according to the shape of each of the nanostructures, the volume and level of the molecules of the derivatives of the nanostructures are different. , On the other hand, changes in the volume of the molecules of derivatives of different nanostructures with the same carbon number as shown below:

$$V_{\text{RDX Nano Tube}} > V_{\text{RDX Nano Cone}} > V_{\text{RDX Ger}} > V_{\text{RDX C20}} > V_{\text{RDX}}$$

Also, the comparison of the level of the molecules of various nanostructure derivatives with the number of carbon is similar to the following:

$$A_{RDX\ Nano\ Tube} > A_{RDX\ Nano\ Cone} > A_{RDX\ Ger} > A_{RDX\ C20} > A_{RDX}$$

Comparing the incremental trend of the specific heat capacity, the volume and surface of the molecules of the derivatives of different nanostructures with the same number of carbon and their coordination, shows that, under the same conditions in terms of molecular mass, increasing the volume and level of the molecule increases the amount of specific heat capacity of the molecule. We know that the specific heat capacity of a CV is the amount of heat that is given to a mole of matter to rise to a temperature of one degree, it is evident that the more energy the material is, the less the specific heat of its CV. Therefore, it is concluded that the molecules of derivatives of different nanostructures with the same number of carbon and the same molecular mass with RDX explosives have a higher volume and surface, the product is less energy efficient. Table (1). Comparison of the values of other thermodynamic parameters studied in this study confirms the results.

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